Inosine 58-63-9 | DTXSID2045993

Model Performance

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Model	I)ata
Widdei	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 217 °C

Global applicability domain: Inside

Local applicability domain index: 3.90e-01

Confidence level: 5.78e-01

Nearest Neighbors from the Training Set

Image not found

Adenosine Measured: 246 Predicted: 236 Image not found

Adenosine Measured: 246 Predicted: 236 Image not found

Fludarabine Measured: 260 Predicted: 243

Image not found

Pentostatin Measured: 220 Predicted: 219 Image not found

6-Methylmercaptopurine

ribonucleoside Measured: 164 Predicted: 178